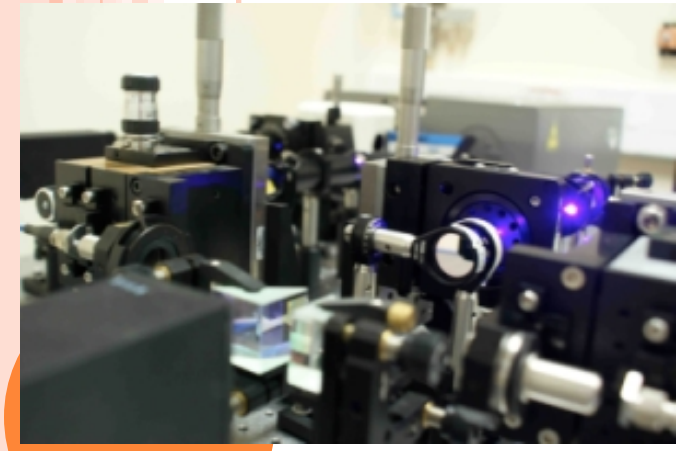
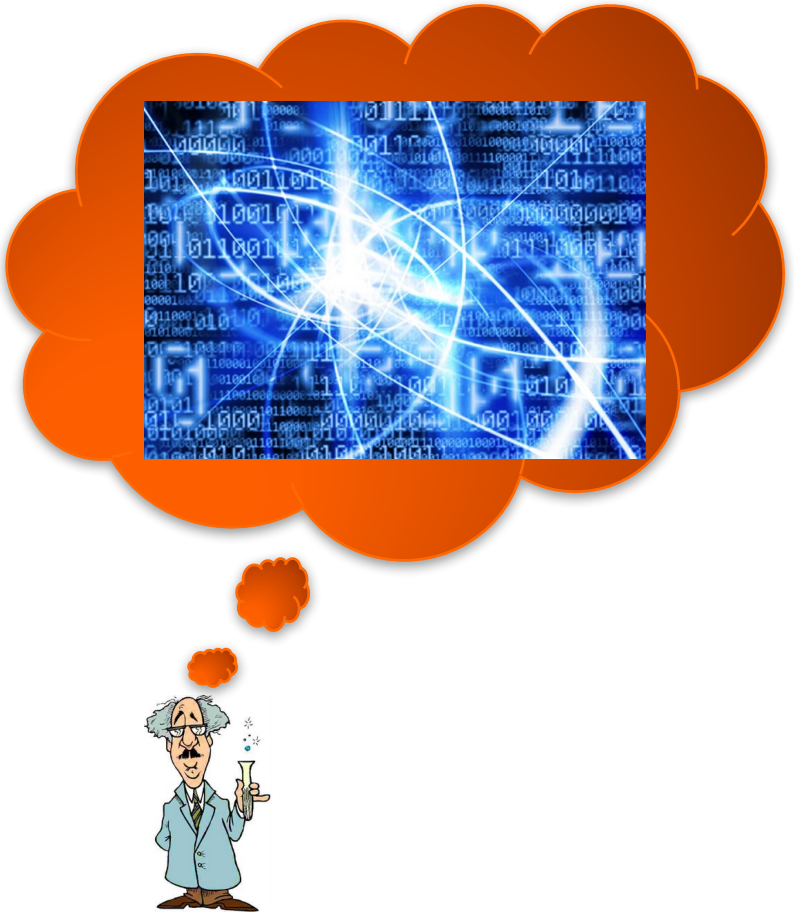
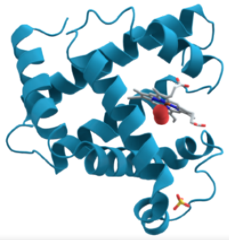
Quantum Computation for Chemistry and Materials



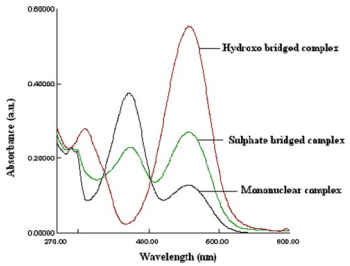


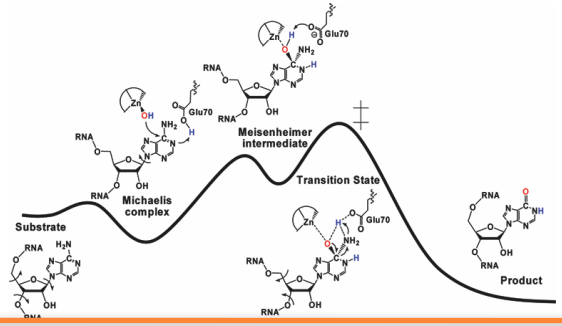
Jarrod R. McClean
Alvarez Fellow - Computational Research Division
Lawrence Berkeley National Laboratory

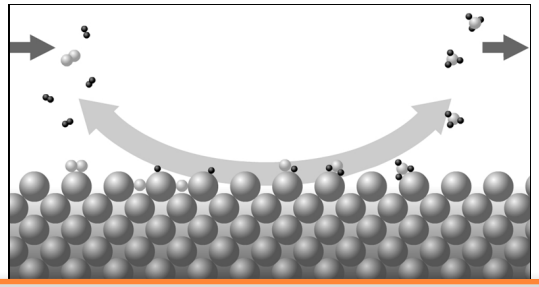
Why Quantum Chemistry?



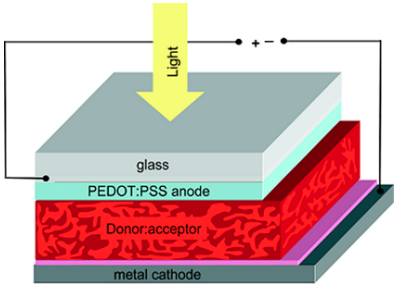
Understanding

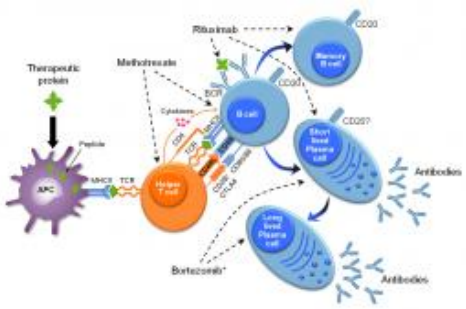






Control

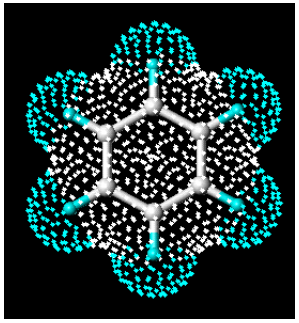




The Electronic Structure Problem

"The underlying physical laws necessary for the mathematical theory of a large part of physics and the whole of chemistry are thus completely known, and the difficulty is only that the exact application of these laws leads to equations much too complicated to be soluble."

-Paul Dirac



$$\mathcal{H}\left|\psi\right\rangle = E\left|\psi\right\rangle$$

Grand solutions from a grand device

$$N_2 + 3\ H_2 \rightarrow 2\ NH_3$$ → Fertilizer

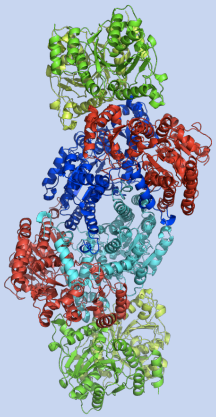
Humans: Haber Process

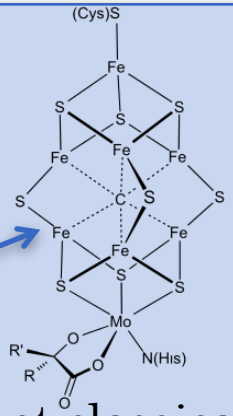
400° C & 200 atm

1-2% of ALL energy on earth, used on Haber process

Nature: Nitrogenase

25° C & 1 atm





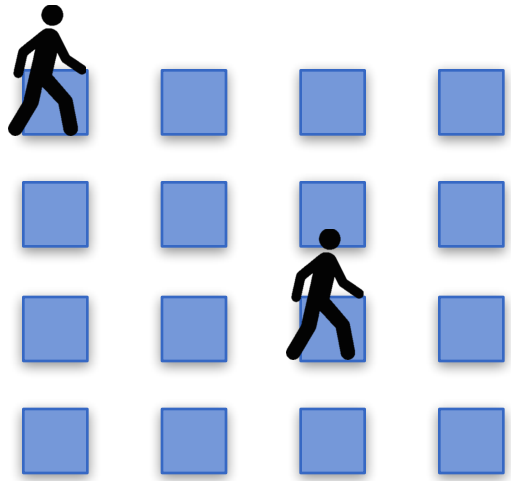
"FeMoco"

Beyond all current classical methods

Both electronic structure and substrate attachment almost totally unknown

Classically – No clear path to accurate solution
Quantum Mechanically – 150-200 logical qubits for solution

Aside: Probability Distributions



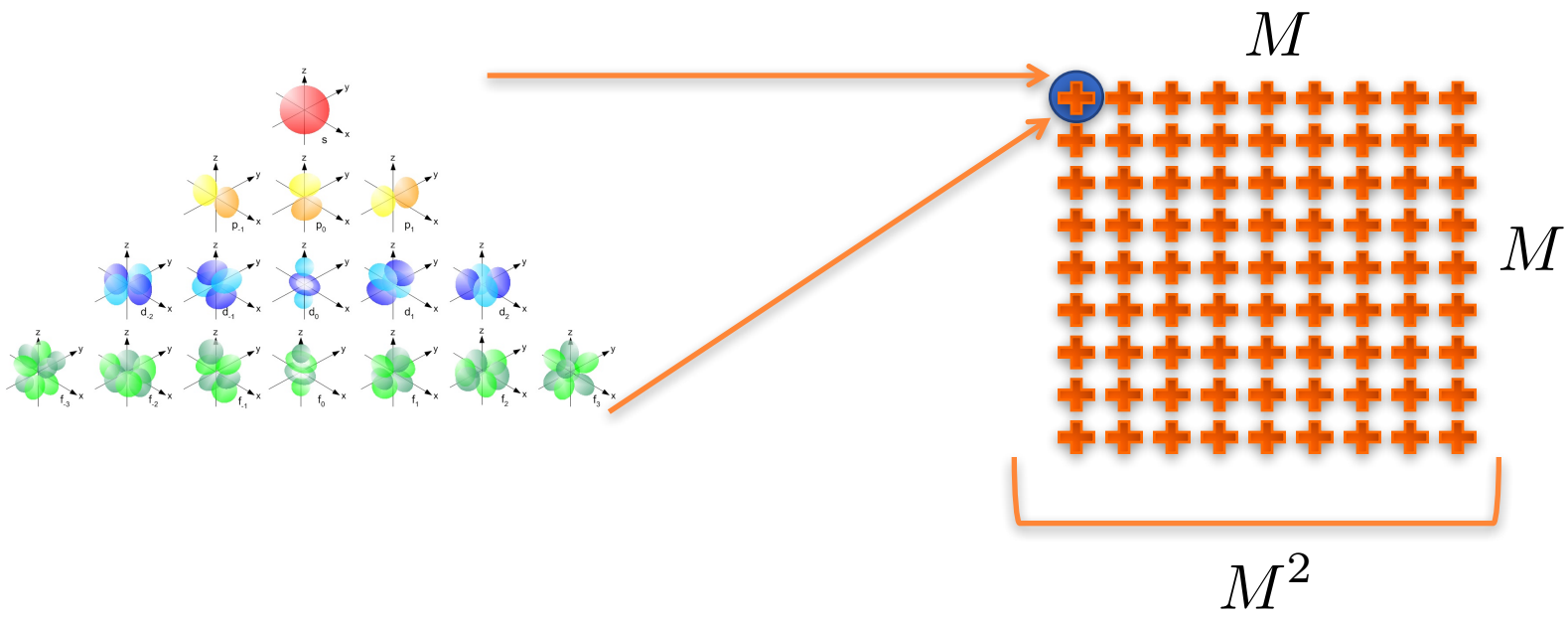
$$P_1(\text{Store}_i) \quad P_2(\text{Store}_j)$$

$$P_{12}(\text{Store}_i, \text{Store}_j) \neq P_1(\text{Store}_i) P_2(\text{Store}_j)$$

$$O(N^P) \qquad O(PN)$$

Technical caveat: our "probability distributions" may be complex valued

The exponential problem



$$D = M^N$$

$$M = 100$$
$$N = 80$$

$$D = 100^{80} = 10^{160}$$

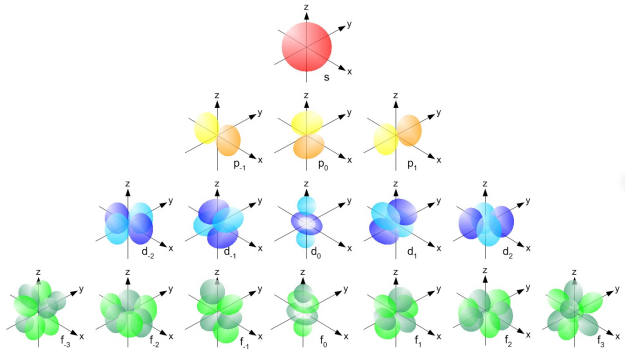
Electrons:

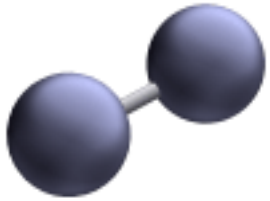
$$D = \begin{pmatrix} M \\ N_\alpha \end{pmatrix} \begin{pmatrix} M \\ N_\beta \end{pmatrix}$$

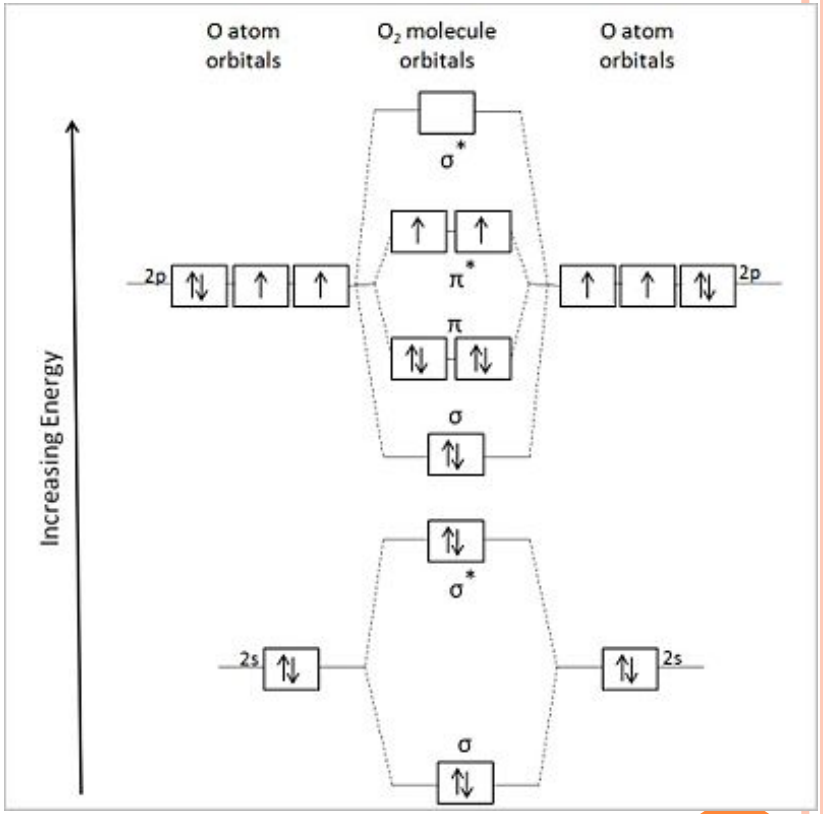
One mole
10^{23}

Particles in universe
10^{80}

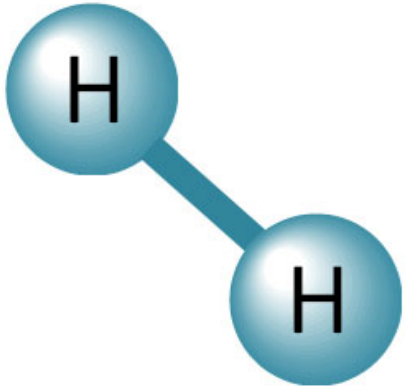
LCAO and Molecular Orbitals

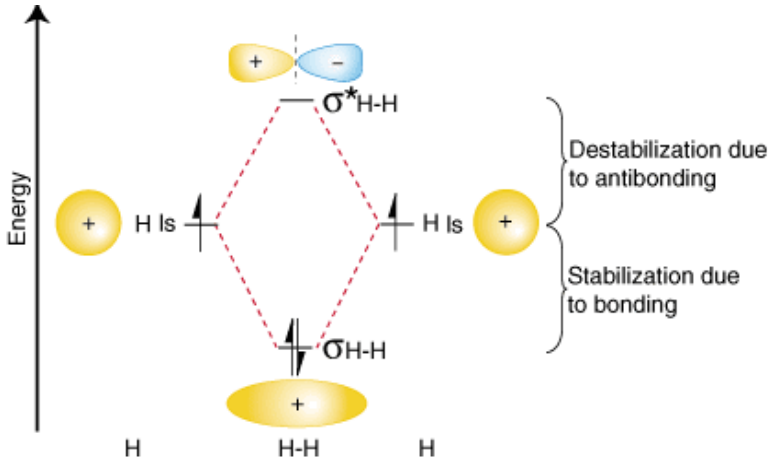






Simple but not good enough





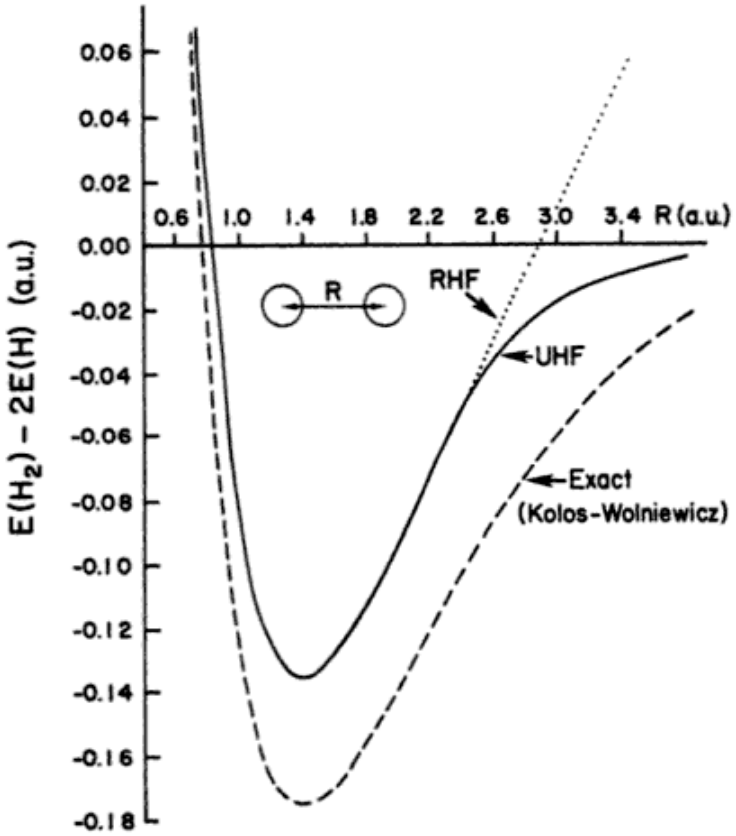
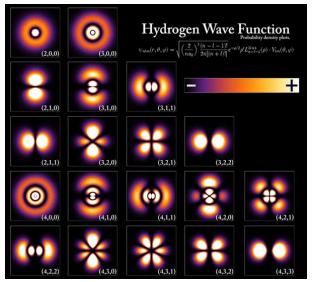


Figure 3.19 6-31G** potential energy curves for H_2.

Classical Pre-Calculations

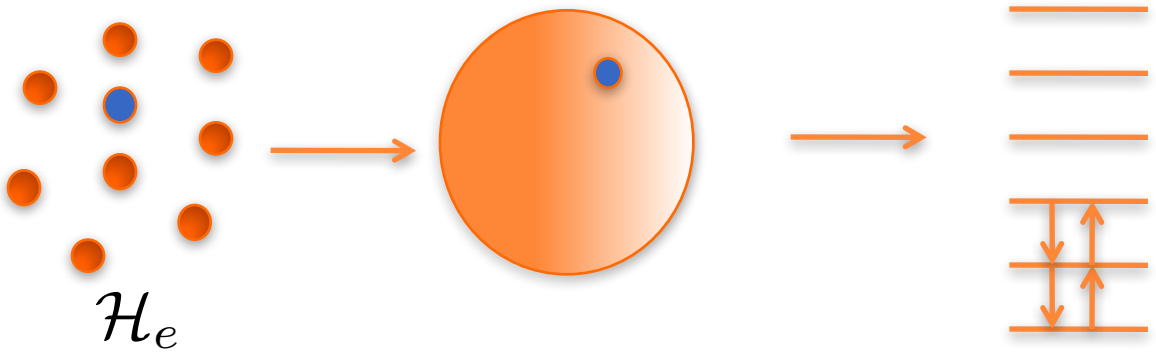
Second-Quantized Electronic Hamiltonian

$$\mathcal{H}_e(R) = h_{pq}(R)\hat{a}_p^\dagger \hat{a}_q + h_{pqrs}(R)\hat{a}_p^\dagger \hat{a}_q^\dagger \hat{a}_r \hat{a}_s$$



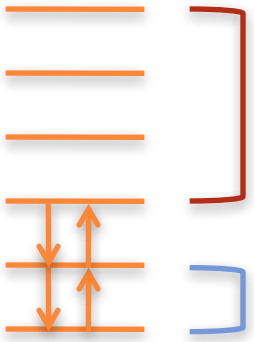
Atom Centered Basis

Hartree-Fock (Mean-Field)



Molecular Orbitals

Beyond the mean Field



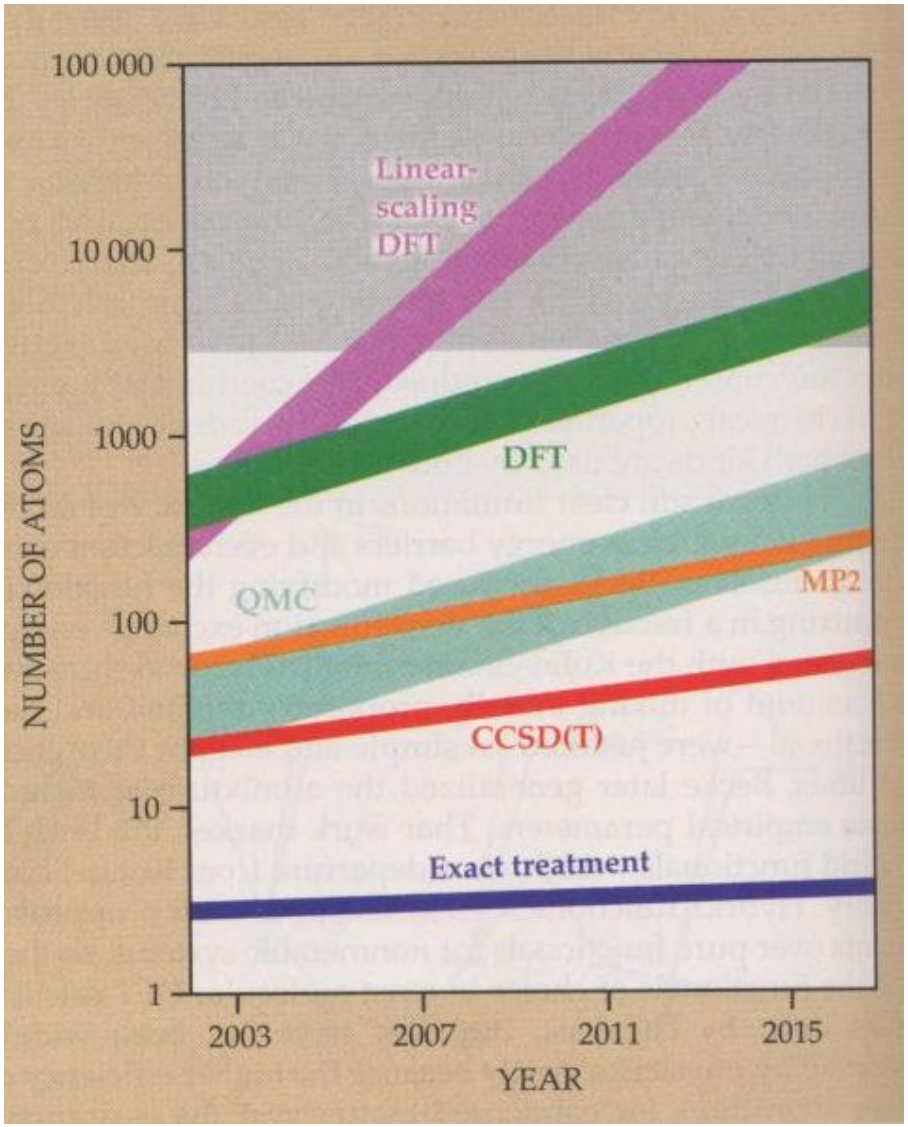
Virtual

Occupied

$$|\Psi\rangle = c_0 \quad + c_1 \quad + c_2 \quad + c_3 \quad \bullet\bullet\bullet$$

$$|\Psi\rangle = \sum_{i_1 i_2 \ldots i_N} c^{i_1 i_2 \ldots i_N} |i_1 i_2 \ldots i_N\rangle$$

Between Mean-Field and Exact



DFT (Density Function Theory): Errors in transition states,
Charge transfer excitations, anions,
Bond breaking

MP2 – Second order perturbation theory,
Good for hydrogen bonding, failing for
Weakly bond systems and bond breaking

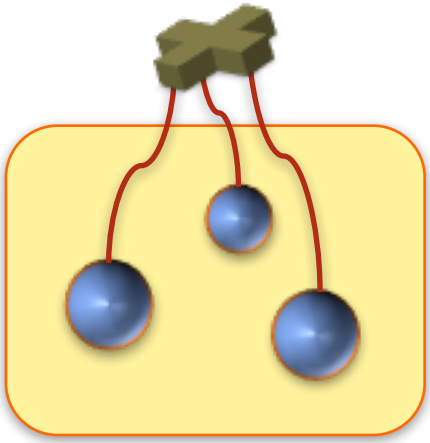
QMC – Quantum Monte Carlo,
Stochastic, accuracy depends on trial function

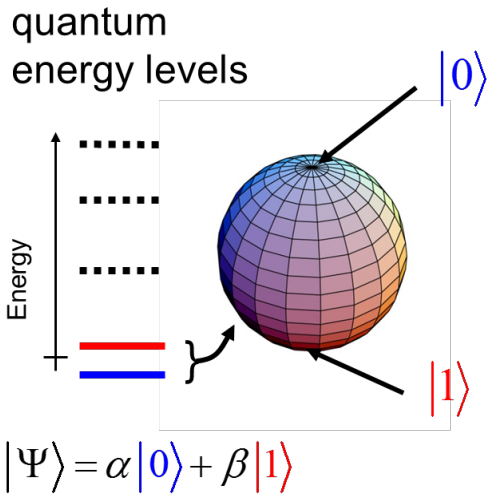
CCSD(T) (Coupled Cluster single doubles excitations with perturbative triples) –
"Gold Standard" for weakly bound systems,
fails for multiple bond breaking

Exact (Full Configuration Interaction)

M. Head-Gordon, M. Artacho,
Physics Today 4 (2008)

Quantum Simulation – The Quantum Advantage





Quantum Simulation

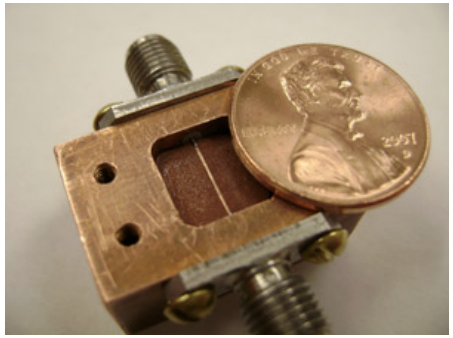
Quantum Computation

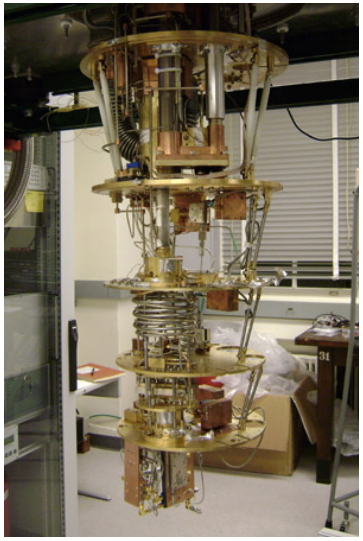
- Factoring Products of Two Large Primes
- Linear Partial Differential Equations
- Solution of Linear Equations

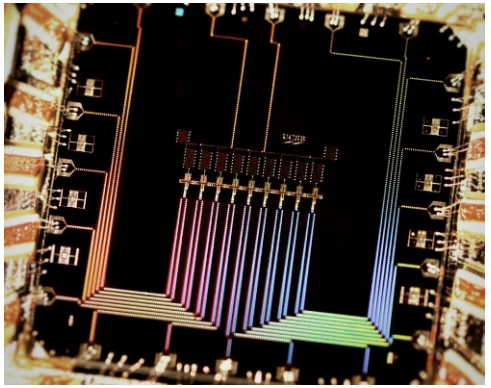
Abstraction

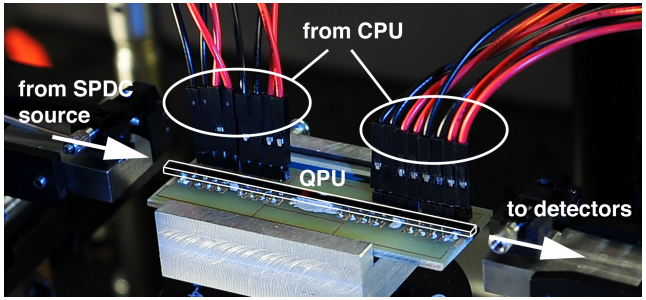
Prep $|\psi\rangle$ → Evolution → Measurement → $\{|\Psi_i\rangle, E_i\}$

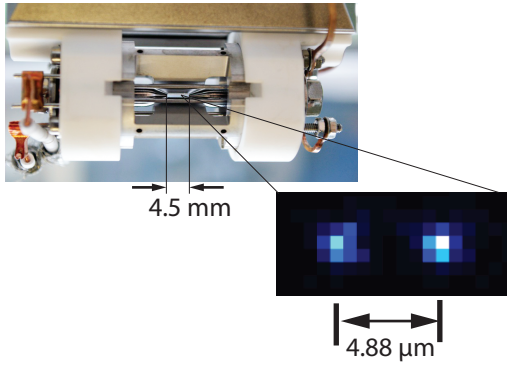
Quantum Hardware



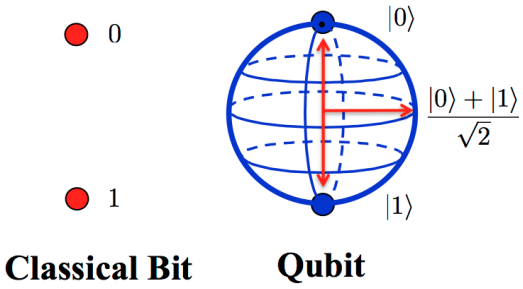


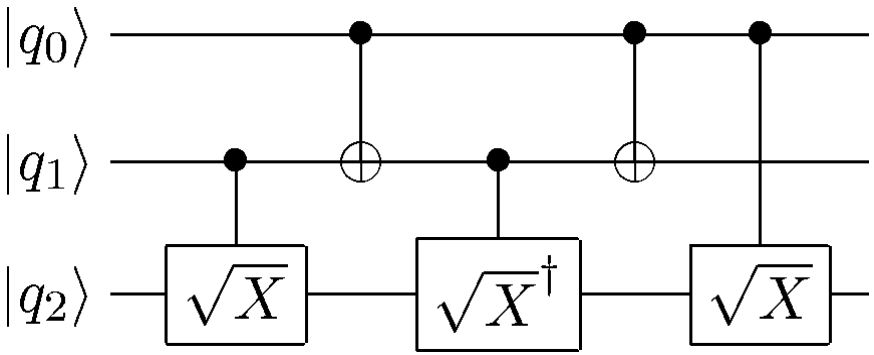






Quantum Computing Abstraction





$$|0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

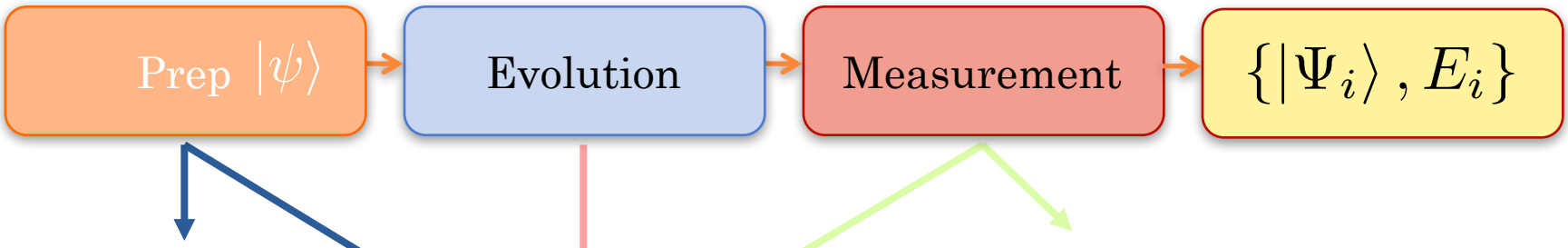
$$|1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

$$X = \mathrm{NOT} = \sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

$$X|0\rangle = |1\rangle$$

$$X|1\rangle = |0\rangle$$

Challenges in Quantum Simulation

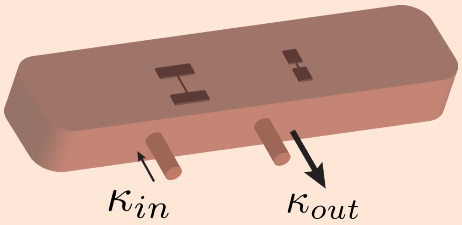


Number of Qubits
+Scalable manufacture
+(N-1) qubit problem

Coherence Time & Fidelity
+Robust control & stable qubits
+Algorithm timescale problem

Information Extraction
+New input/output spec
+Full readout loses advantage

Better Hardware



Co-Design Better Algorithms

Previous: Coherence time flexible – VQE

Future:

- Improved coherence time flexibility, novel property extraction, and demonstration – QSE
- Qubit number flexible algorithms and larger demonstrations

A New Co-design Perspective

Currently: Given a task, design quantum circuit (or computer) to perform it.

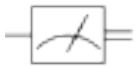
Problem: General or optimal solution can require millions of gates.

Alternative: Given a task and the current architecture, find the best solution possible.

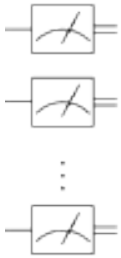
Peruzzo†, **McClean†**, Shadbolt, Yung, Zhou, Love, Aspuru-Guzik, O'Brien. *Nature Communications*, 5 (4213):1– 7, 2014.
† Equal Contribution by authors

Easy Task For A Quantum Computer

$\langle \sigma_i^z \rangle$



$\langle \sigma_1^z \sigma_2^z \ldots . \sigma_n^z \rangle$



- Efficient to perform on any prepared quantum state
- In general, it may be very hard to calculate this expectation value for a classical representation, containing an exponential number of configurations

$$|\Psi\rangle = \sum_{i_1 i_2 \ldots i_N} c^{i_1 i_2 \ldots i_N} |i_1 i_2 \ldots i_N\rangle$$

Back to Basics

Variational Formulation: Minimize $\langle \Psi | H | \Psi \rangle$

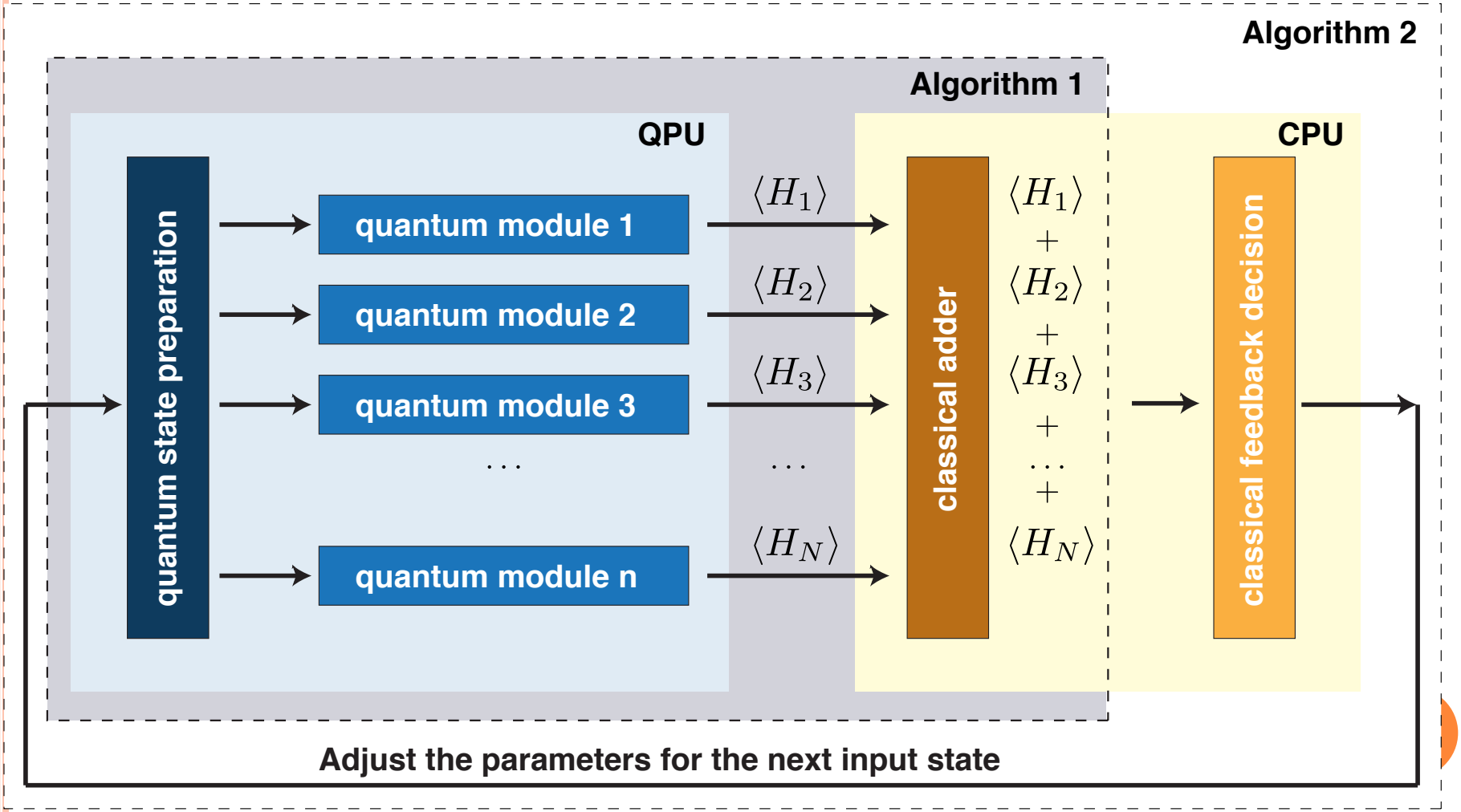
Decompose as: $\mathcal{H} = h^i_\alpha \sigma^i_\alpha + h^{ij}_{\alpha\beta} \sigma^i_\alpha \sigma^j_\beta + h^{ijk}_{\alpha\beta\gamma} \sigma^i_\alpha \sigma^j_\beta \sigma^k_\gamma + \ldots$

By Linearity: $\langle \psi | \mathcal{H} | \psi \rangle \equiv \langle \mathcal{H} \rangle = \mathcal{H} = h^i_\alpha \langle \sigma^i_\alpha \rangle + h^{ij}_{\alpha\beta} \langle \sigma^i_\alpha \sigma^j_\beta \rangle + h^{ijk}_{\alpha\beta\gamma} \langle \sigma^i_\alpha \sigma^j_\beta \sigma^k_\gamma \rangle + \ldots$

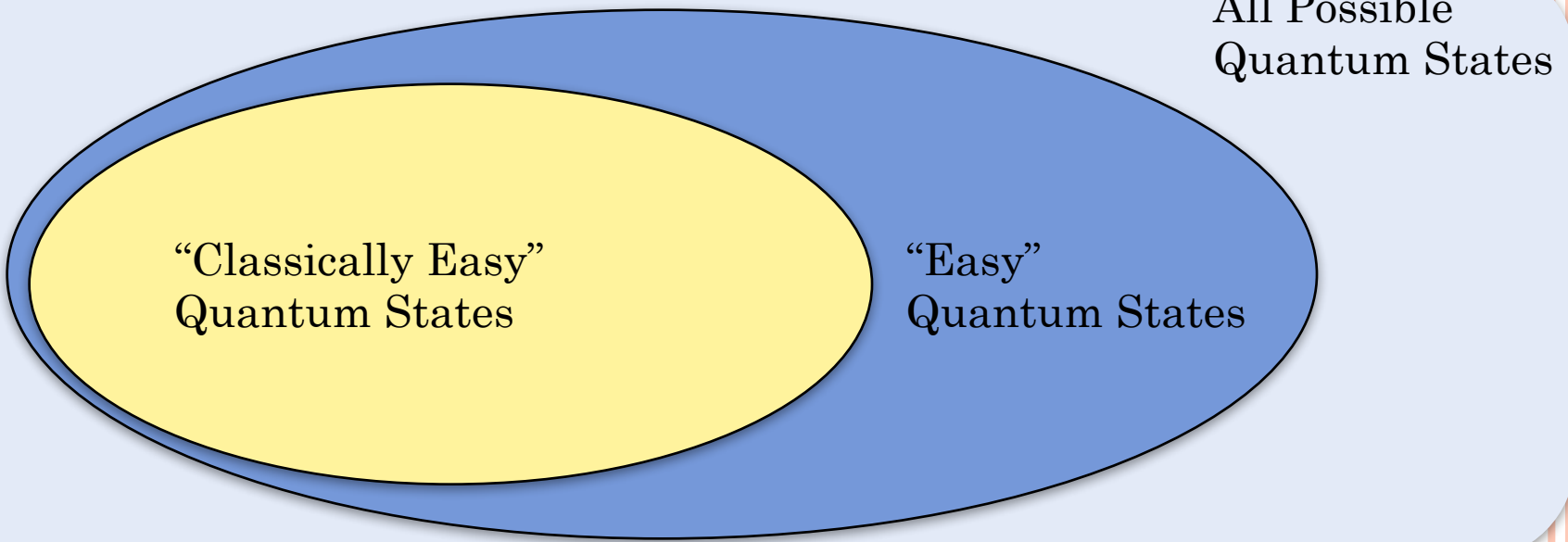
Easy for a Quantum Computer: $\langle \sigma^i_\alpha \sigma^j_\beta \sigma^k_\gamma \ldots \rangle$ → Easy for a Classical Computer: $+, \times \rightarrow \langle H \rangle$

Suggests Hybrid Scheme:
- Parameterize Quantum State with Classical Experimental Parameters
- Compute Averages using Quantum Computer
- Update State Using Classical Minimization Algorithm (e.g. Nelder-Mead)

Computational Algorithm

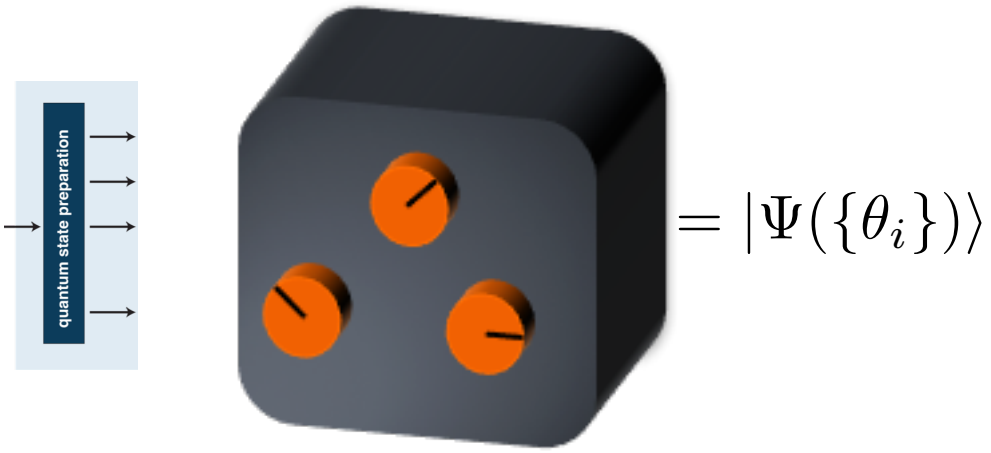


Essentials of a quantum Advantage



State Ansatz

Quantum Hardware Ansatz: "Any Quantum Device with knobs"



$$= |\Psi(\{\theta_i\})\rangle$$

Use the complexity of your device to your advantage

Coherence time requirements are set by the device, not algorithm

Unitary Coupled Cluster Ansatz

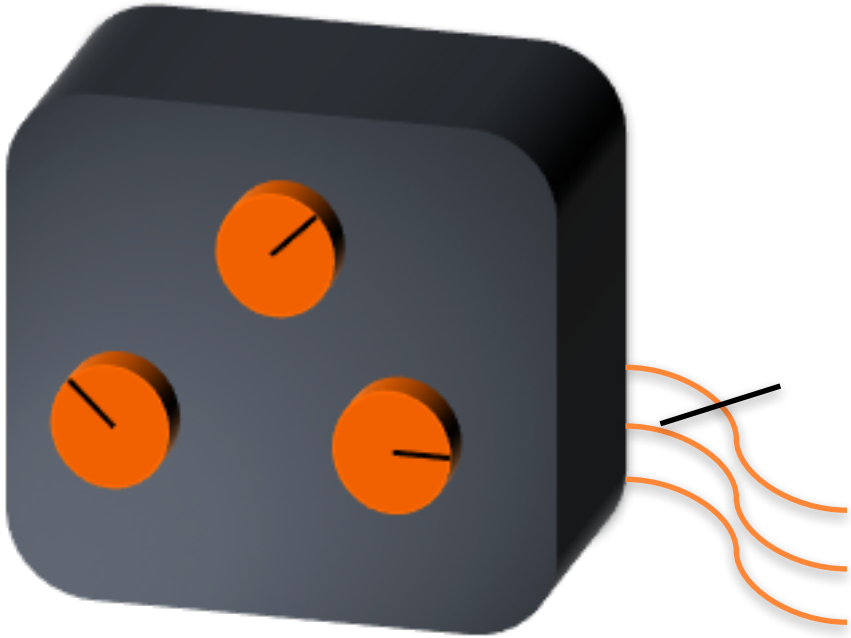
$$|\Psi\rangle = e^{T-T^\dagger}|\Phi_0\rangle$$

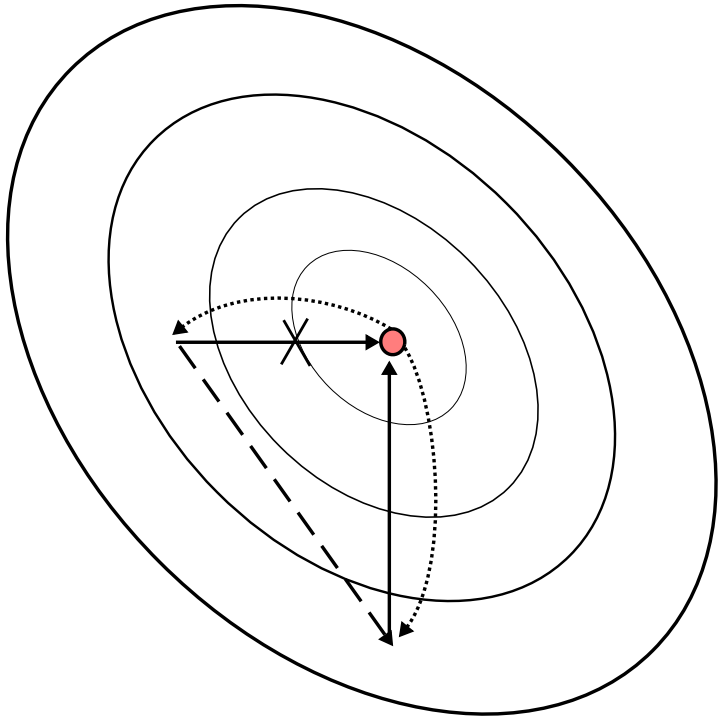
(A-)diabatic State Preparation

$$H(s) = [1 - A(s)]H_i + A(s)H_p$$

$$A(0) = 0$$
$$A(1) = 1$$

Variational Error Suppression





McClean, J.R., Romero, J., Babbush, R, Aspuru-Guzik, A.
"The theory of variational hybrid quantum-classical algorithms"
ArXiv e-prints (2015) arXiv: 1509.04279 [quant-ph]

"Killer App": Quantum Chemistry

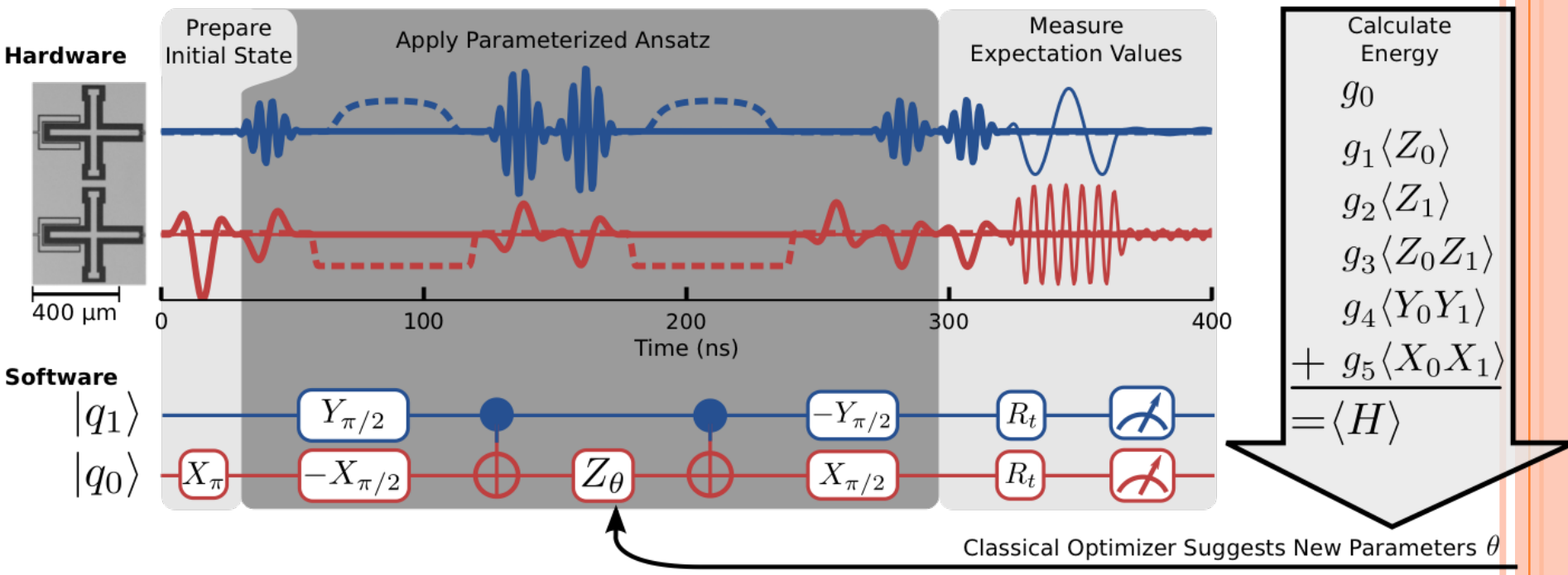
Current experimental literature state of the art:

	Quantum Phase Estimation	Variational Quantum Eigensolver
H_2	NMR (Jiangfeng Du et al. 2010)	
	Photonic chips (B. P. Lanyon et al. 2010)	
	Superconducting qubits (P. J. J. O'Malley, Babbush, **McClean** et al. 2015)	Superconducting qubits (P. J. J. O'Malley, Babbush, **McClean** et al. 2015)
HeH^+	NV centers (Ya Wang et al. 2015)	Photonic chips (Peruzzo, **McClean** et al. 2014)
		Trapped ions (Yangchao Shen et al. 2015)

Theoretical and Algorithmic (2016):

[1] **McClean** et al., N. J. Phys 18 023023 (2016)
[2] Sawaya and **McClean** et al, JCTC - in press (2016)
[3] **McClean,** Schwartz, Carter, de Jong ArXiv:1603.05681 [quant-ph] (2016)
[4] Reiher et al. ArXiv:1605.03590 [quant-ph] (2016)
[5] Babbush et al. N. J. Phys. 18 (3), 033032 (2016)

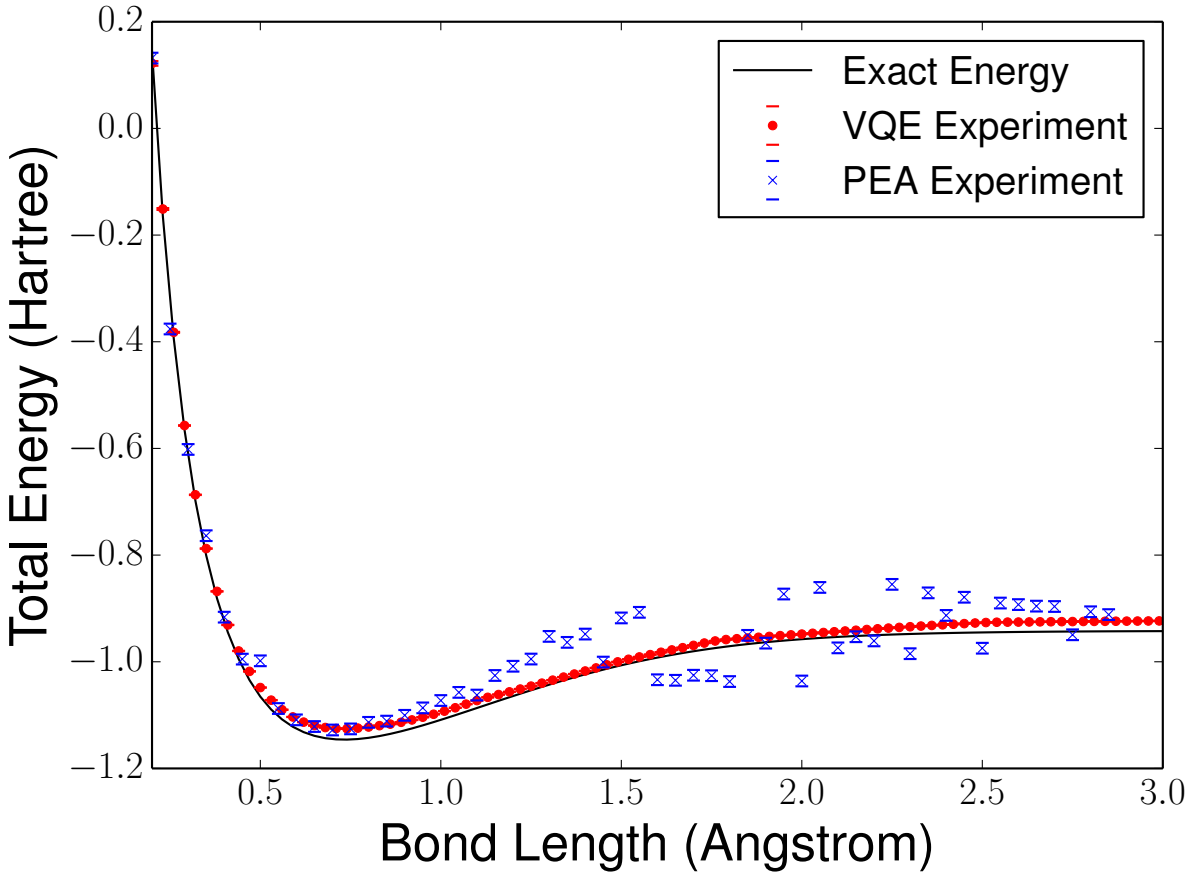
Scalable Simulation of Molecular Energies in Superconducting Qubits



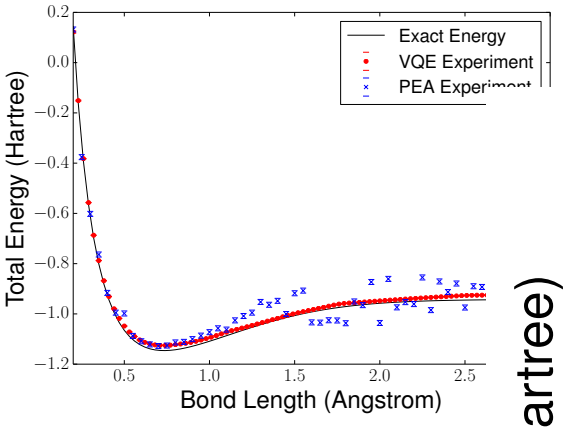
Google

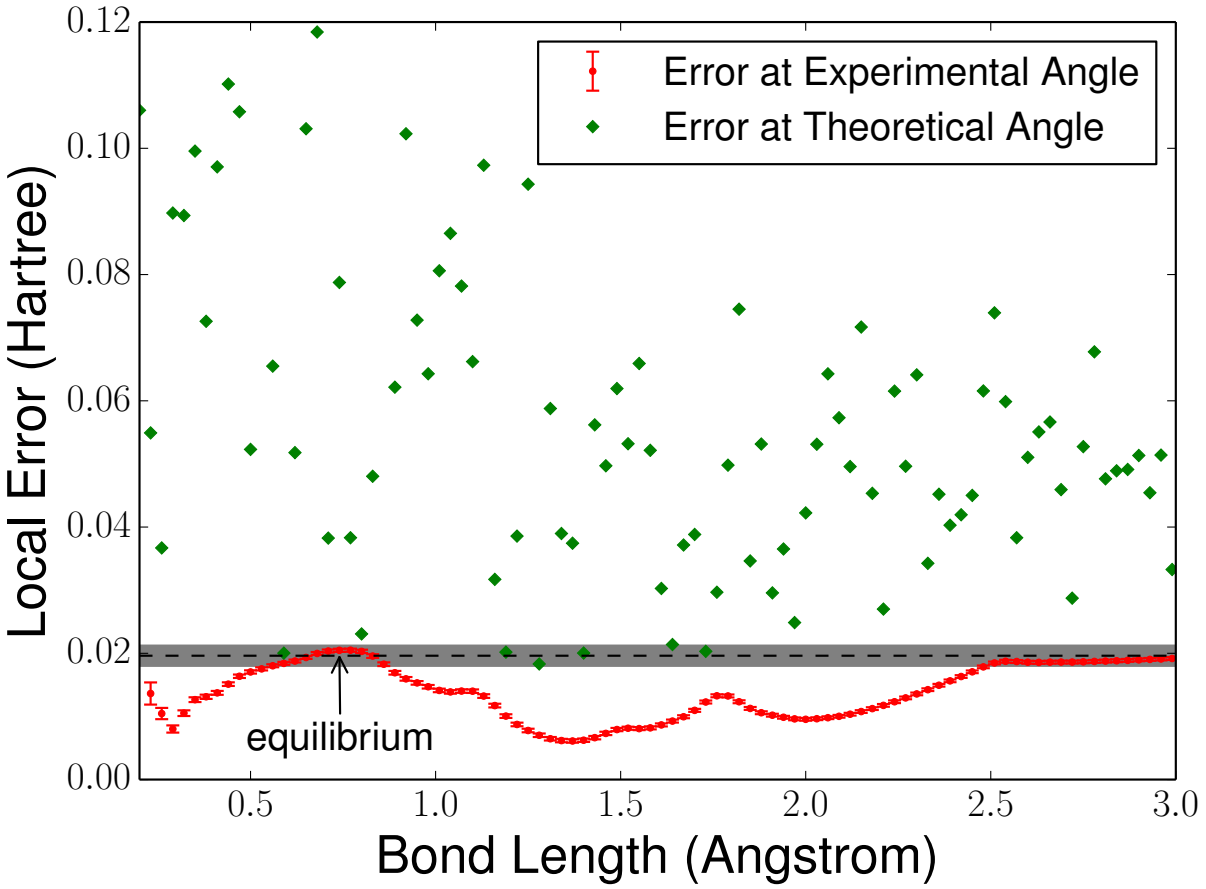
P.J.J. O'Malley, R. Babbush,…, J.R. McClean et al.
"Scalable Simulation of Molecular Energies"
ArXiv e-prints (2015) arXiv: 1512.06860 [quant-ph]

Variational Error Suppression



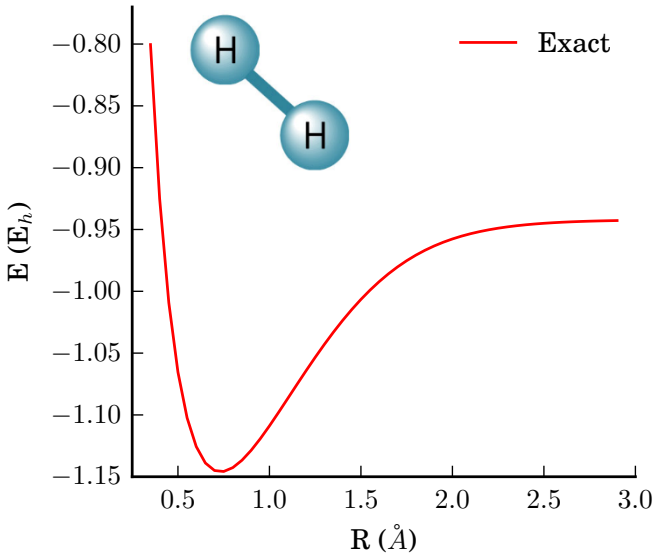
Variational Error Suppression





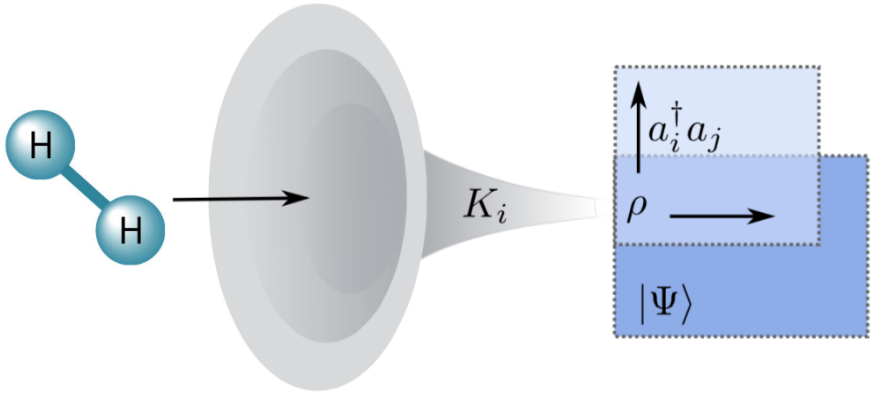
Quantum Subspace Expansion (QSE)

Quantum State on Quantum Device



Expand to Linear Response (LR) Subspace

Extra Quantum Measurements



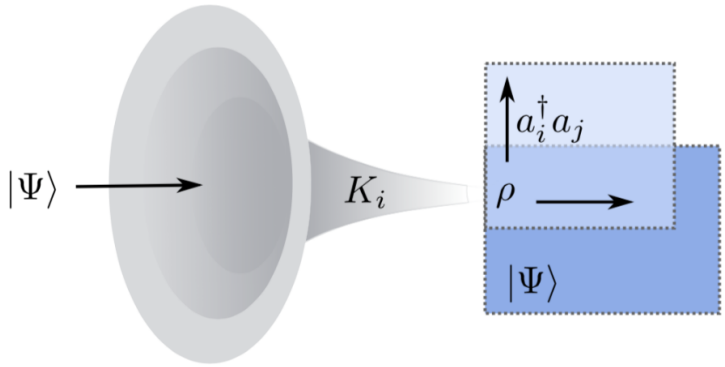
Classical Generalized Eigenvalue Problem

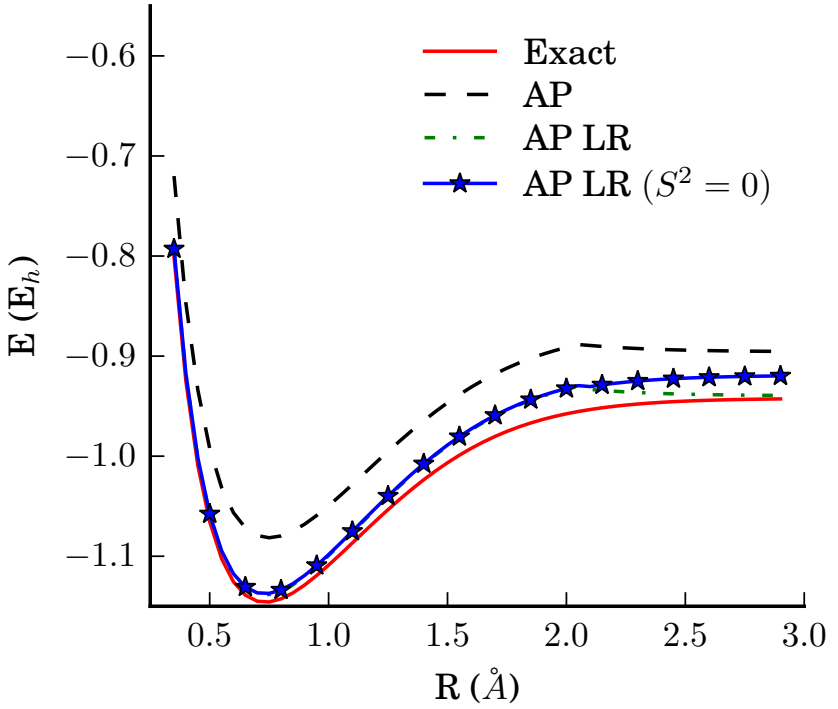
$$HC = SCE$$

Excited State Energy and Properties

Hybrid Quantum-Classical Hierarchy for Mitigation of Decoherence and Determination of Excited States
McClean, J.R., Schwartz, M.E, Carter, J., de Jong, W.A.
ArXiv:1603.05681 [quant-ph] (2016)

Expansion Mitigates Noise





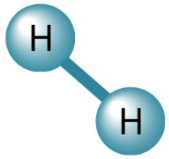
Subspace expansion restores symmetry

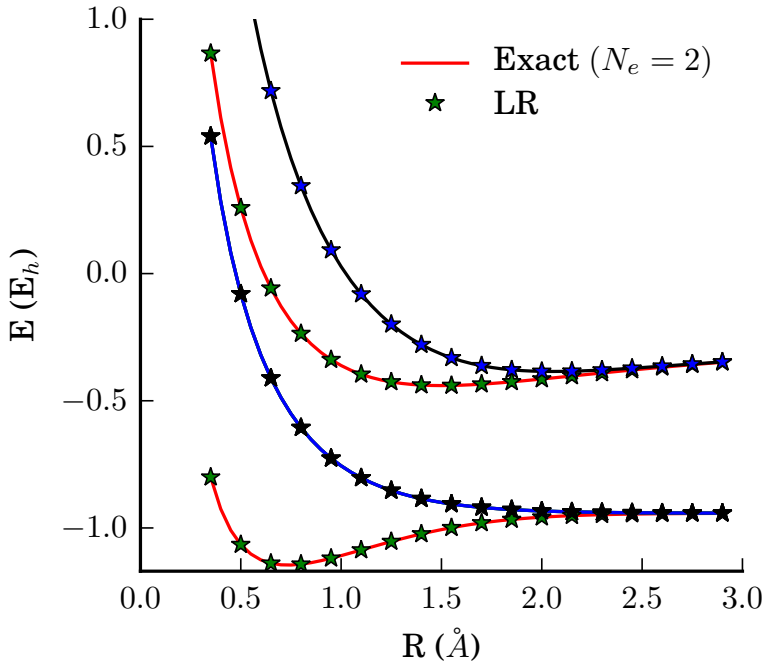
$$OC = SC\Lambda$$

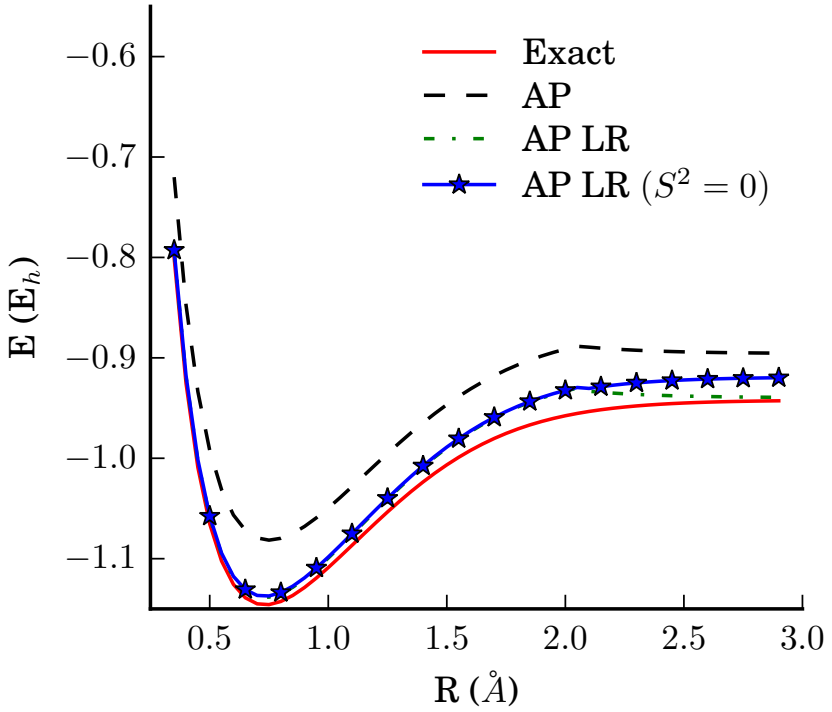
$\tilde{H}_{kl}^{ij}$ (Hamiltonian projected into symmetry subspace)

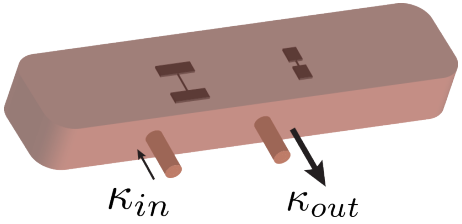
Excited States and Error Suppression

$$HC = SCE$$

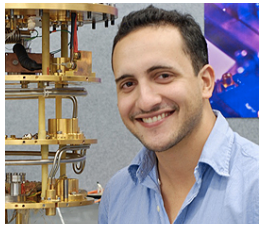




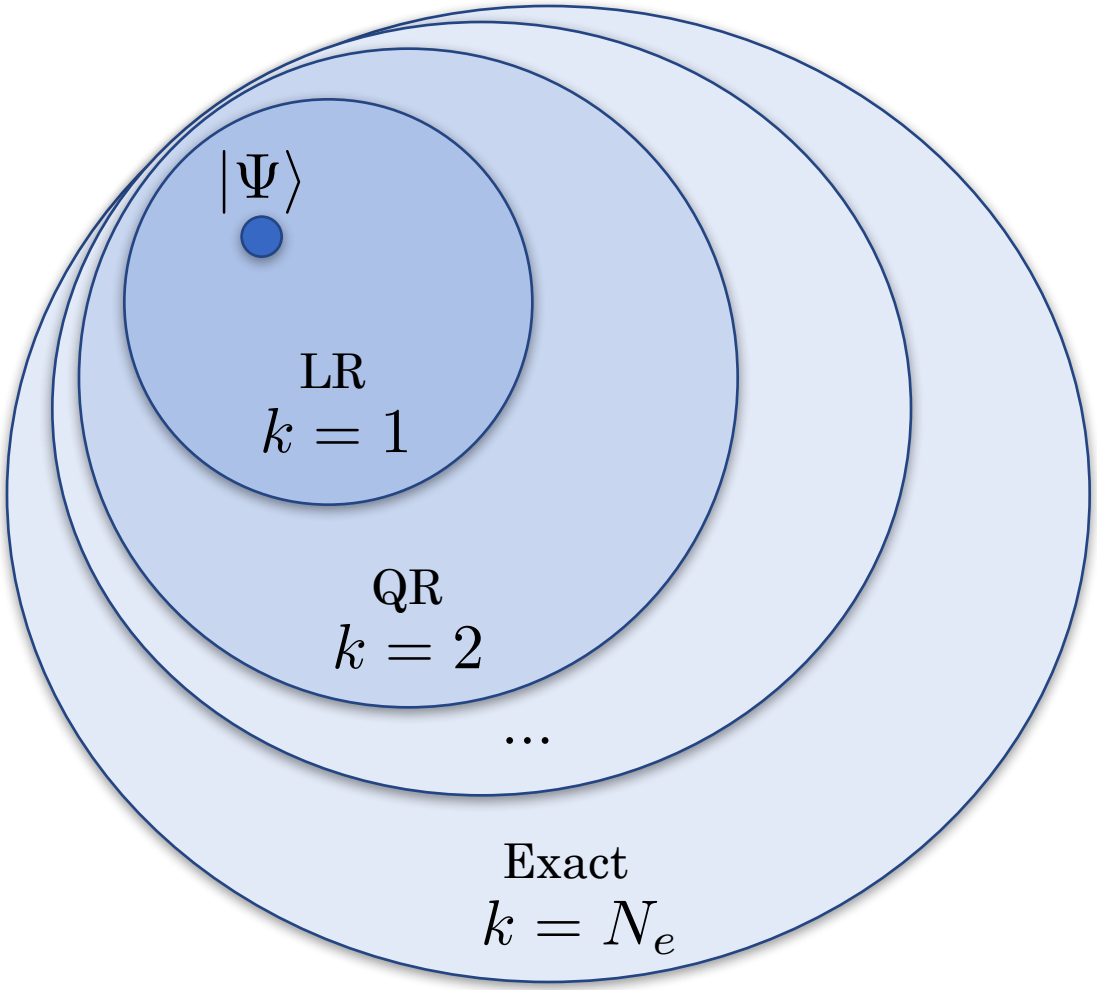




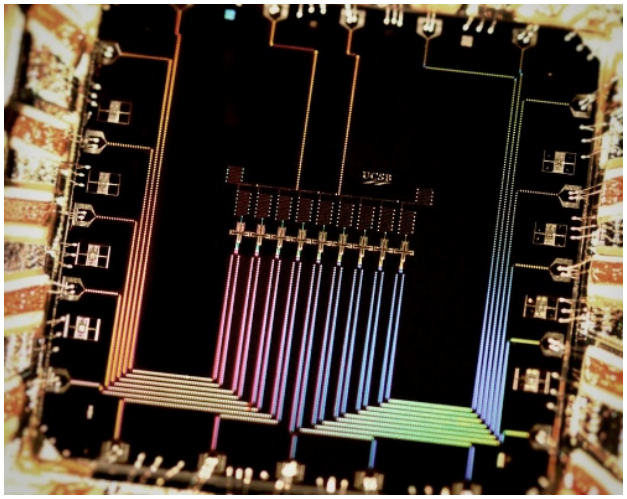
Experimental demonstration in progress!



Expansion forms exact hierarchy



Why Now?



*http://web.physics.ucsb.edu/~martinisgroup/

Google

Microsoft

intel

IBM

D:wave
The Quantum Computing Company™

U.S. DEPARTMENT OF ENERGY

Los Alamos
NATIONAL LABORATORY
EST. 1943

HRL LABORATORIES

BERKELEY LAB

LOCKHEED MARTIN

Grand solutions from a grand device

$$N_2 + 3\ H_2 \rightarrow 2\ NH_3$$ → Fertilizer

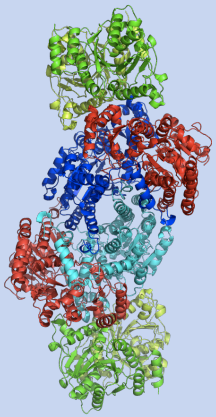
Humans: Haber Process

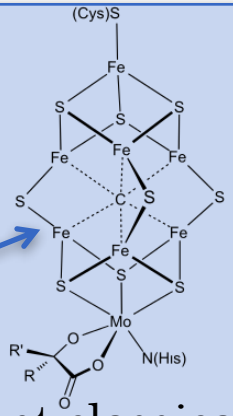
400° C & 200 atm

1-2% of ALL energy on earth, used on Haber process

Nature: Nitrogenase

25° C & 1 atm





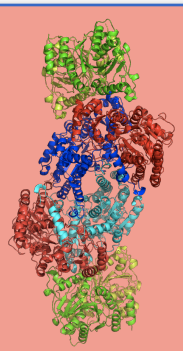
"FeMoco"

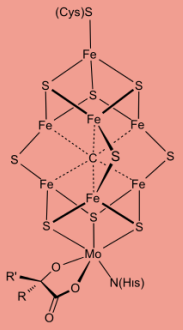
Beyond all current classical methods

Both electronic structure and substrate attachment almost totally unknown

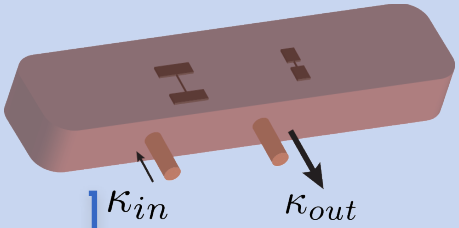
Classically – No clear path to accurate solution
Quantum Mechanically – 150-200 logical qubits for solution

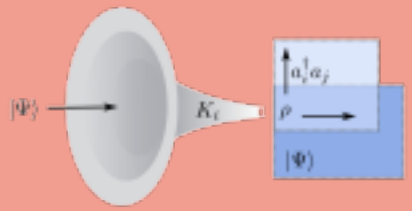
Summary

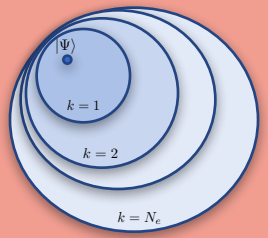




150-200 Logical Qubits







Acknowledgements

LBNL:
Wibe A. De Jong
Jonathan Carter

Harvard University:
Alán Aspuru-Guzik

Google Quantum AI Labs
Ryan Babbush
Peter O'Malley
John Martinis

UC Berkeley:
Irfan Siddiqi
Mollie Schwartz